Electron-atom ionization near the Bethe ridge: revision of plane wave first-order theories

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Abstract. We consider electron impact single ionization of an atom at large energy-momentum transfer in the nearly Bethe-ridge kinematics. For evaluation of the ionization amplitude, a plane wave Born series is employed. A regularization procedure is utilized in circumventing typical divergence problems associated with the higher-order Born terms. The regularized Born series for the ionization amplitude is derived. On this basis, renormalized analogs of the traditional plane wave Born and impulse approximations are developed. These renormalized first-order models resemble the traditional plane wave impulse approximation with a modified Gamow factor. Numerical results using different approximations are presented and analyzed for the case of electron-hydrogen ionization. The present theoretical consideration can be important for absolute measurements.

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1. Introduction

Single ionization by electron impact (or (e,2e) collision) at large energy-momentum transfer in the nearly Bethe-ridge kinematics, where the recoil ion momentum is small compared with the transferred one, constitutes a powerful spectroscopic tool for exploring electronic structure of atomic systems [1, 2, 3, 4]. This (e,2e) method is often referred to as the Electron Momentum Spectroscopy (EMS) [1, 2]. Theoretical grounds of the EMS exploit domination of the lowest-order term, such as given by the plane wave Born or impulse approximation (PWBA or PWIA), when treating the ionization amplitude perturbatively and using plane waves for description of the incident and outgoing electron states. Formally, the ratio of the higher-order and lowest-order Born terms behaves as $\propto E_0^{-1/2}$, where E_0 is the incident electron energy, and hence one might expect the lowest-order term to prevail at high values of E_0. However, on the energy shell the plane wave higher-order terms are given by divergent integrals [5], which are due to so-called Coulomb singularities of the transition operator [6, 7, 8]. Therefore, for drawing conclusions on the validity of the PWBA model, one should cope with the problem of divergences of the corresponding perturbation series.

The Born series follows from the Lippmann-Schwinger equation which has a noncompact kernel. However, in the case of short-range potentials, the noncompactness of the kernel does not prevent from calculating matrix elements of the Born series. For the purpose of a mathematically correct formulation, Faddeev proposed to reduce the Lippmann-Schwinger equation to a system of three coupled equations with compact kernels [9, 10]. This system leads to the Born-Faddeev series where two-particle amplitudes depending on three arguments (the relative-motion energy and incoming/outgoing momenta) appear instead of the corresponding potentials. The higher-order Born-Faddeev terms contain the two-particle amplitudes which in general are off-shell, i.e. their arguments do not necessarily obey the energy-momentum relations for free particles. The lowest-order Born-Faddeev term, given by a half-on-shell two-particle amplitude, yields the usual PWIA.

In the case of Coulomb potentials Faddeev's reduction does not offer mathematical advantages, since the kernel remains noncompact [6, 10]. This is a consequence of the fact that the plane wave states do not obey the correct asymptotic behavior for the Coulomb breakup. Thus, the resultant Born-Faddeev series contains divergent terms and, like the PWBA case, the validity of the PWIA model is questionable. At the same time, plane waves are usually a convenient and handy mathematical tool for calculating the Born and Born-Faddeev series. And as far as the corresponding higher-order terms diverge on the energy shell, one must resort to a regularization procedure which removes the artificial, unphysical problem of divergences. Further, one must find a relation between the regularized perturbation series and the exact ionization amplitude. Only then, a perturbative treatment of the ionization amplitude can be developed in a physically consistent manner.

The objective of this work is to revise the traditional PWBA and PWIA models

in the light of the fact that these first-order theories ignore the divergence problem associated with the higher-order contributions to the ionization amplitude. The present theoretical analysis is based on the results of [5], where a practical recipe for regularization of the plane wave Born series was proposed, and those of Shablov *et al* [7, 8, 10], who established a relation between the exact ionization amplitude and the unphysical plane wave Lippmann-Schwinger one in the on-shell limit. We proceed from the Born series, since, as mentioned above, Faddeev's reduction is not of benefit in the case of Coulomb potentials and hence may lead to methodological confusion. After regularizing the Born series, one can formulate renormalized analogs of the traditional PWBA and PWIA models. These analogs resemble the traditional PWIA model with a modified Gamow factor. As shown below, the modified Gamow factor depends on the choice of a regularization procedure and therefore it is not uniquely determined. This feature permits, in principle, to choose such version of the Gamow factor that efficiently incorporates higher-order effects ignored by the traditional first-order models. The above points are addressed in the consideration that follows and are illustrated with numerical results.

Section 2 of this paper delivers a general formulation for the (e,2e) reaction on an atom. In section 3, specific Born approximations are formulated using a regularized Born series. Section 4 is devoted to the impulse approximation theory in the context of the regularization formalism. The numerical results for the case of electron-hydrogen ionization are presented and discussed in section 5 and the conclusions are drawn in section 6. The atomic units (au) $e = \hbar = m_e = 1$ are used throughout unless otherwise stated.

2. General formulation

We specify the momenta of the incident, scattered and ejected electrons by $\boldsymbol{k}_0$, $\boldsymbol{k}_s$ and $\boldsymbol{k}_e$, respectively. The corresponding energies are denoted by E_0, E_s and E_e. The initial atomic and the final ionic states are specified by their respective wavefunctions Φ_i^Z, Φ_f^{Z-1}, where Z designates the nuclear charge, and energies ε_i, ε_f. The rate of the (e,2e) reaction is characterized by the triple differential cross section (TDCS)

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_s \mathrm{d}\Omega_e \mathrm{d}E_e} = \frac{k_e k_s}{(2\pi)^5 k_0} \left(\frac{1}{4}|T_s + T_e|^2 + \frac{3}{4}|T_s - T_e|^2 \right). \tag{1}$$

Here the directions of the outgoing electron momenta are specified by the solid angles Ω_s and Ω_e. The amplitude T_s (T_e) corresponds to the situation where the scattered electron has the momentum $\boldsymbol{k}_s$ ($\boldsymbol{k}_e$). The so-called capture amplitude is ignored, since we consider such kinematical regimes where the capture of the incident electron accompanied with ejection of two atomic electrons having the momenta $\boldsymbol{k}_s$ and $\boldsymbol{k}_e$ is negligible. In equation (1) a sum (average) over unresolved ionic (atomic) states is assumed.

The amplitude is given by (below we focus on the amplitude T_s omitting its index)

$$T = \langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e) \rangle, \tag{2}$$

where V_i is the potential between the incident electron and the atom. The initial asymptotic state $|\boldsymbol{k}_0\Phi_i^Z\rangle \equiv |\boldsymbol{k}_0\rangle \otimes |\Phi_i^Z\rangle$, where $|\boldsymbol{k}_0\rangle$ is the plane wave state for the incident electron, satisfies the Schrödinger equation

$$(H - V_i - E)|\boldsymbol{k}_0\Phi_i^Z\rangle = 0,$$

where H is the full projectile-atom Hamiltonian and E is the total energy:

$$E = E_s + E_e + \varepsilon_f = E_0 + \varepsilon_i.$$

The total scattering state $|\Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle$ takes account of all interactions between the final-state fragments. It satisfies the Schrödinger equation

$$(H - E)|\Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle = 0$$

and obeys the proper Coulomb asymptotics, whose specificity is due to a long-range character of the interactions between the final-state fragments.

2.1. The plane wave Born series

To avoid confusion, we will use a tilde for marking the Lippmann-Schwinger analogs of the physical quantities that have been introduced in the preceding subsection (such as the amplitude T and the total scattering state $|\Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle$). In the context of the Lippmann-Schwinger formalism which employs plane wave states for treating asymptotically free particles, the total scattering state is sought as a solution to the equation

$$|\tilde{\Psi}_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle = |\boldsymbol{k}_s\boldsymbol{k}_e\Phi_f^{Z-1}\rangle + G_0^-(E)V|\tilde{\Psi}_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle, \qquad V = V_s + V_e + V_{se}, \tag{3}$$

where V_s, V_e, and V_{se} are the electron-ion and electron-electron potentials, respectively. The Green's operator $G_0^-(E)$ is given by

$$G_0^-(E) = (E - H + V - \mathrm{i}0)^{-1}. \tag{4}$$

The final asymptotic state $|\boldsymbol{k}_s\boldsymbol{k}_e\Phi_f^{Z-1}\rangle \equiv |\boldsymbol{k}_s\rangle \otimes |\boldsymbol{k}_e\rangle \otimes |\Phi_f^{Z-1}\rangle$, where $|\boldsymbol{k}_s\rangle$ and $|\boldsymbol{k}_e\rangle$ are, respectively, the plane wave states for the scattered and ejected electrons, satisfies the Schrödinger equation

$$(H - V - E)|\boldsymbol{k}_s\boldsymbol{k}_e\Phi_f^{Z-1}\rangle = 0.$$

Equation (3) can be presented in the equivalent form

$$|\tilde{\Psi}_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle = [1 + G^-(E)V]|\boldsymbol{k}_s\boldsymbol{k}_e\Phi_f^{Z-1}\rangle \tag{5}$$

where $G^-(E) = (E - H - \mathrm{i}0)^{-1}$ is the full Green's operator.

Substitution of (5) into (2) generates the plane wave perturbation series

$$\tilde{T} = \sum_{n=0}^{\infty} \tilde{T}^{(n)} \qquad \text{where } \tilde{T}^{(n)} = \langle \boldsymbol{k}_0\Phi_i^Z|V_i[G_0^-(E)V]^n|\boldsymbol{k}_s\boldsymbol{k}_e\Phi_f^{Z-1}\rangle, \tag{6}$$

which is traditionally referred to as the Born series. Here the $n = 0$ term amounts to the usual PWBA

$$\tilde{T}^{(0)} \equiv T^{\text{PWBA}} = \langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1} \rangle. \tag{7}$$

All other (higher-order) Born terms $\tilde{T}^{(n)}$ and the sum of these terms are divergent (see [5] and Appendix A for details). These observations are not novel and are due to a well-known fact that the plane wave states do not obey the asymptotic conditions peculiar to break-up Coulomb scattering. Thus, equation (6) gives an unphysical result and hence it can not be employed for a perturbative treatment of the correct, physical amplitude (2). In addition, the validity of the traditional PWBA model (7) can not be based upon equation (6).

2.2. The off-shell Born series

The situation changes if we consider the Born series (6) off the energy shell, i.e. when $E \neq E_s + E_e + \varepsilon_f$. Setting $E - E_s - E_e - \varepsilon_f = \Delta > 0$, we have

$$\tilde{T}(\Delta) = \sum_{n=0}^{\infty} \tilde{T}^{(n)}(\Delta) \equiv T^{\text{PWBA}} + \sum_{n=1}^{\infty} \tilde{T}^{(n)}(\Delta) \qquad (\tilde{T}^{(n)}(0) \equiv \tilde{T}^{(n)}), \tag{8}$$

where all the higher-order Born terms are finite [5] (see also Appendix A). If the value of the off-shell parameter Δ approaches the on-shell case $\Delta = 0$, the Born series (8) exhibits a typical Coulomb singularity $\tilde{T}(\Delta) \propto \Delta^{-\text{i}\eta}$ [6, 8, 10], where η is a total Sommerfeld parameter:

$$\eta = \eta_s + \eta_e + \eta_{se} \qquad (\eta_s = -k_s^{-1}, \ \eta_e = -k_e^{-1}, \ \text{and} \ \eta_{se} = |\boldsymbol{k}_s - \boldsymbol{k}_e|^{-1}).$$

The physical amplitude (2) is derived from (8) in the following manner [7, 8, 10]:

$$T = \frac{\exp(-\frac{1}{2}\pi\eta - \text{i}A)}{\Gamma(1 + \text{i}\eta)} \lim_{\Delta \to 0} \Delta^{\text{i}\eta} \tilde{T}(\Delta), \tag{9}$$

where

$$A = \eta_s \ln(2k_s^2) + \eta_e \ln(2k_e^2) + \eta_{se} \ln |\boldsymbol{k}_s - \boldsymbol{k}_e|^2$$

is the Dollard phase [11]. Note that in the on-shell limit $\Delta \to 0$ the divergent factor $\Delta^{\text{i}\eta}$ compensates for the singularity of $\tilde{T}(\Delta)$. In the next section we show how the calculation scheme based on equation (9) can be implemented in practice through regularization of the Born series.

3. Born approximations

For taking the on-shell limit $\Delta \to 0$ in equation (9), it is convenient to have $\Delta^{-\text{i}\eta}$ factored out in the off-shell Born series (8). This can be fulfilled by means of a regularization procedure (see Appendix B). As a result, we obtain the amplitude (9) in the factorized form

$$T = \mathcal{R}\tilde{T}_{\mathcal{R}}, \qquad \tilde{T}_{\mathcal{R}} = \sum_{n=0}^{\infty} \tilde{T}_{\mathcal{R}}^{(n)} \equiv T^{\text{PWBA}} + \sum_{n=1}^{\infty} \tilde{T}_{\mathcal{R}}^{(n)}, \tag{10}$$

where $\tilde{T}_{\mathcal{R}}^{(n)}$ is the regularized on-shell Born term and $\mathcal{R}$ is a regularization function†, such that $\mathcal{R} = 1$ if $\eta_s = \eta_e = \eta_{se} = 0$.

In contrast to (6), the result (10) allows to develop a perturbative treatment of the physical amplitude. However, when truncating the regularized on-shell Born series $\tilde{T}_{\mathcal{R}}$ to a finite number of terms, there is an uncertainty associated with the choice of a regularization procedure. Namely, while

$$\mathcal{R}\tilde{T}_{\mathcal{R}} = \mathcal{R}'\tilde{T}_{\mathcal{R}'},$$

where $\mathcal{R}'$ and $\tilde{T}_{\mathcal{R}'}$ are due to an alternative regularization procedure (see Appendix B for details), in general

$$\mathcal{R}' \sum_{n=0}^{N} \tilde{T}_{\mathcal{R}'}^{(n)} \neq \mathcal{R} \sum_{n=0}^{N} \tilde{T}_{\mathcal{R}}^{(n)}.$$

In particular, the lowest-order approximation ($N = 0$) to the amplitude (10) assumes the form

$$T_{\mathcal{R}}^{\text{PWBA}} = \mathcal{R}\tilde{T}_{\mathcal{R}}^{(0)} \equiv \mathcal{R}T^{\text{PWBA}} \tag{11}$$

that depends on the choice of a regularization procedure/function. These observations are reminiscent of the situation that one encounters in quantum electrodynamics, when regularizing a series of Feynman's diagrams. Drawing an analogy with that situation, one can speak of a renormalization group which is formed by the regularization procedures in the present case. Therefore we will refer to equation (11) as a renormalized PWBA (RPWBA).

In this work we develop the Born series for the physical amplitude (2) in a manner similar to equation (6), that is

$$T = \sum_{n=0}^{\infty} T^{(n)}, \tag{12}$$

where $T^{(n)}$ is given by the nth-order term of the Maclaurin series expansion of the exact amplitude T with respect to the two-particle Sommerfeld parameters η_s, η_e, and η_{se}. It can be deduced from (10) that

$$T^{(n)} = \tilde{T}_{\mathcal{R}=1}^{(n)}, \tag{13}$$

where $\tilde{T}_{\mathcal{R}=1}^{(n)}$ corresponds to the specific regularization procedure which yields $\mathcal{R} = 1$ for any values of η_s, η_e, and η_{se} (see Appendix B).

According to (13), the lowest-order term of (12) amounts to the usual PWBA result (7):

$$T^{(0)} \equiv T^{\text{PWBA}} = \langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1} \rangle. \tag{14}$$

The plane wave second Born approximation (PWB2), which is usually of practical value for estimating the applicability of the PWBA, is then given by

$$T^{\text{PWB2}} = T^{(0)} + T^{(1)} = T^{\text{PWBA}} + \tilde{T}_{\mathcal{R}=1}^{(1)}. \tag{15}$$

† Hereafter $\mathcal{R}$ refers to an arbitrary regularization procedure/function unless otherwise specified.

Using (9), this is equivalent to

$$T^{\mathrm{PWB2}} = \left(1 - \frac{\pi\eta}{2} - \mathrm{i}A + \mathrm{i}\gamma\eta\right) T^{\mathrm{PWBA}} + \lim_{\Delta\to 0}[\tilde{T}^{(1)}(\Delta) + \mathrm{i}\eta T^{\mathrm{PWBA}} \ln\Delta], \tag{16}$$

where $\gamma = 0.577216$ is the Euler constant.

4. Impulse approximations

4.1. The usual theory

Near the Bethe ridge the (e,2e) process can be modelled as a binary encounter between the projectile electron and the electron that is ejected from the atom [1]. The PWIA theory formulates this picture mathematically. Within the Lippmann-Schwinger approach (6) it is expressed as follows:

$$\tilde{T}^{\mathrm{PWIA}} = \sum_{n=0}^{\infty} \tilde{T}_{se}^{(n)}, \qquad \text{where } \tilde{T}_{se}^{(n)} = \langle \boldsymbol{k}_0 \Phi_i^Z | V_{se}[G_0^-(E)V_{se}]^n | \boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1} \rangle. \tag{17}$$

As in the case of (6), the $n \geq 1$ terms and the sum of these terms are divergent. We can remedy this defect in order to obtain a correct, convergent counterpart of (17). For this purpose we use the result (10), assuming that $V_i = V = V_{se}$ and, accordingly, $\eta_s = \eta_e = 0$. Thus one derives the physical counterpart of (17) as

$$T^{\mathrm{PWIA}} = \mathcal{R}_{se} \tilde{t}_{\mathcal{R}} F_{if}(\boldsymbol{q}) = \tau F_{if}(\boldsymbol{q}) \qquad (\mathcal{R}_{se} = \mathcal{R}|_{\eta_s=\eta_e=0}), \tag{18}$$

where $\boldsymbol{q} = \boldsymbol{k}_s + \boldsymbol{k}_e - \boldsymbol{k}_0$ is opposite to the recoil ion momentum and $F_{if}(\boldsymbol{q}) = \langle \Phi_i^Z | \Phi_f^{Z-1} \boldsymbol{q} \rangle$ is the so-called structure amplitude [1]. $\tilde{t}_{\mathcal{R}}$ is the regularized Lippmann-Schwinger half-on-shell amplitude for ee-scattering [5] and τ is the exact half-on-shell ee-scattering amplitude [12, 13]:

$$\tau = \tau\{\boldsymbol{k}_0 - \tfrac{1}{2}(\boldsymbol{k}_s + \boldsymbol{k}_e), \tfrac{1}{2}(\boldsymbol{k}_s - \boldsymbol{k}_e); [\tfrac{1}{2}(\boldsymbol{k}_s - \boldsymbol{k}_e)]^2\}.$$

The result (18) is irrespective of the choice of a regularization procedure, since $\mathcal{R}_{se}\tilde{t}_{\mathcal{R}} = \mathcal{R}'_{se}\tilde{t}_{\mathcal{R}'}$. Note that equation (18) is a corner-stone of the usual PWIA theory of (e,2e) reactions on atoms [1, 2].

4.2. A renormalized theory

While there is nothing wrong in the above derivation of the traditional PWIA result, it can be noticed that at the starting point (17) we have focused on the purely electron-electron part of (6) and thereby we have ignored the remaining part which is also divergent. Methodologically, one should apply the binary-encounter approximation to the regularized Lippmann-Schwinger amplitude $\tilde{T}_{\mathcal{R}}$ (see (10)) which, in contrast to (6), is free of divergences. The electron-electron component of $\tilde{T}_{\mathcal{R}}$ is given by the regularized Lippmann-Schwinger amplitude $\tilde{t}_{\mathcal{R}}$ for ee-scattering (see (18)). Using (10) and (18), the PWIA to the physical amplitude T is then given by

$$T_{\mathcal{R}}^{\mathrm{PWIA}} = \mathcal{R}\tilde{t}_{\mathcal{R}} F_{if}(\boldsymbol{q}) = (\mathcal{R}/\mathcal{R}_{se})\tau F_{if}(\boldsymbol{q}). \tag{19}$$

Since in general $\mathcal{R}/\mathcal{R}_{se} \neq \mathcal{R}'/\mathcal{R}'_{se}$, the PWIA amplitude (19) is determined by the choice of a regularization procedure. In particular, the specific case $\mathcal{R}/\mathcal{R}_{se} = 1$ amounts to the traditional PWIA (18). As far as the choice of a regularization procedure is a matter of taste, equation (19) offers an infinite number of alternatives. This fact has the following general consequence: there is no *a priori* PWIA model in the case of (e,2e) reactions on atoms. By analogy with the RPWBA case (11), the approximation (19) will be referred to as a renormalized PWIA (RPWIA).

4.3. TDCS and the Gamow factor

Within the traditional PWIA model (18) the TDCS (1) is expressed as [1]

$$\frac{\mathrm{d}^3\sigma^{\mathrm{PWIA}}}{\mathrm{d}\Omega_s\mathrm{d}\Omega_e\mathrm{d}E_e} = \frac{k_sk_e}{2\pi^3k_0}\frac{\mathcal{G}(\eta_{se})}{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}$$
$$\times \left[1 + \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^4} - \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^2}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^2}\cos\left(\eta_{se}\ln\frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|}\right)\right]$$
$$\times \sum^{(\mathrm{av})}|F_{if}(\boldsymbol{q})|^2, \tag{20}$$

where $\sum^{(\mathrm{av})}$ denotes the average over initial-state and sum over final-state degeneracies, and $\mathcal{G}(\eta_{se})$ is the so-called Gamow factor [14]:

$$\mathcal{G}(\eta_{se}) = |\exp(-\tfrac{1}{2}\pi\eta_{se})\Gamma(1 - \mathrm{i}\eta_{se})|^2 = \frac{2\pi\eta_{se}}{\mathrm{e}^{2\pi\eta_{se}} - 1}. \tag{21}$$

In the case of the RPWIA model (19) the expression for TDCS depends on the explicit form of the regularization function $\mathcal{R}$. In this work we inspect the following form:

$$\mathcal{R} = \exp(-\tfrac{1}{2}\pi\eta)\Gamma(1 - \mathrm{i}\eta) \qquad \text{and consequently} \quad \mathcal{R}_{se} = \exp(-\tfrac{1}{2}\pi\eta_{se})\Gamma(1 - \mathrm{i}\eta_{se}). \tag{22}$$

Substitution of (19) and (22) into (1) yields

$$\frac{\mathrm{d}^3\sigma^{\mathrm{RPWIA}}}{\mathrm{d}\Omega_s\mathrm{d}\Omega_e\mathrm{d}E_e} = \frac{k_sk_e}{2\pi^3k_0}\frac{\mathcal{G}(\eta)}{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}$$
$$\times \left[1 + \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^4} - \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^2}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^2}\cos\left(\eta_{se}\ln\frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|}\right)\right]$$
$$\times \sum^{(\mathrm{av})}|F_{if}(\boldsymbol{q})|^2, \tag{23}$$

with the modified Gamow factor

$$\mathcal{G}(\eta) = \frac{2\pi\eta}{\mathrm{e}^{2\pi\eta} - 1}. \tag{24}$$

As can be deduced, the RPWIA result (23) differs from the traditional PWIA one (20) only in the expression for the Gamow factor. In contrast to (21), the modified Gamow factor (24) treats the final-state particle pairs on equal footing. It should be noted that the same result as (24) is obtained using the first-order model introduced by Shablov *et al* [7] on the basis of the formalism of regularization Coulomb operators, and it can be traced down to the idea of effective charges proposed by Peterkop [15]. The influences of the traditional and modified Gamow factors on TDCS are examined in the next section, where we present the corresponding numerical results.

Using the RPWBA model (11) and equation (22), in the binary-encounter approximation ($V_i = V_{se}$) we get

$$\frac{\mathrm{d}^3\sigma^{\mathrm{RPWBA}}}{\mathrm{d}\Omega_s\mathrm{d}\Omega_e\mathrm{d}E_e} = \mathcal{G}(\eta)\frac{\mathrm{d}^3\sigma^{\mathrm{PWBA}}}{\mathrm{d}\Omega_s\mathrm{d}\Omega_e\mathrm{d}E_e}, \tag{25}$$

where the traditional PWBA result is given by [1]

$$\frac{\mathrm{d}^3\sigma^{\mathrm{PWBA}}}{\mathrm{d}\Omega_s\mathrm{d}\Omega_e\mathrm{d}E_e} = \frac{k_s k_e}{2\pi^3 k_0}\frac{1}{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}\left[1 + \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^4}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^4} - \frac{|\boldsymbol{k}_0 - \boldsymbol{k}_s|^2}{|\boldsymbol{k}_0 - \boldsymbol{k}_e|^2}\right]\sum^{(\mathrm{av})}|F_{if}(\boldsymbol{q})|^2. \tag{26}$$

It can be noticed that in symmetric kinematics ($E_s = E_e$, $|\boldsymbol{k}_0 - \boldsymbol{k}_s| = |\boldsymbol{k}_0 - \boldsymbol{k}_e|$), which is usually the case of the EMS experiments (see [1, 3, 4] and references therein), the TDCS given by equation (25) is identical to that given by equation (23).

5. Numerical realization

In this section we present numerical results for an archetypical case, namely the (e,2e) reaction on a hydrogen atom. The symmetric setup $E_s = E_e$ and $\theta_s = \theta_e = 45°$ is inspected, where the polar electron angles θ_s and θ_e are measured with respect to the direction of the incident electron momentum. In the considered setup the TDCS is usually studied as a function of $q = |\boldsymbol{q}|$ (see (17)) whose value is varied in noncoplanar geometry by varying the value of the relative azimuthal angle $\Delta\phi_{se} = \phi_s - \phi_e$, where ϕ_s (ϕ_e) is the azimuthal angle of the scattered (ejected) electron. The minimal value of q corresponds then to the symmetric coplanar case ($|\Delta\phi_{se}| = \pi$), where the incident and outgoing electron momenta are in the same plane.

We focus on high energy values ($E_s = E_e \gtrsim 1$ keV) which closely meet the Bethe-ridge and binary-encounter criteria. In the absence of the corresponding EMS measurements, particularly those performed on an absolute scale, the results of the traditional and renormalized first-order treatments are compared with those of the PWB2 calculations and those of the Brauner-Briggs-Klar (BBK) model [16], a representative of nonperturbative treatments. The PWB2 calculations have been carried out in accordance with (16), where the on-shell limit has been taken analytically using the regularization procedure described in Appendix B. The regularized PWB2 integrals have been performed numerically following the method developed in [17].

In the BBK model the final state in (2) is given by

$$|\Psi^-_{\mathrm{BBK}}(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle = |\varphi^-(\boldsymbol{k}_s)\rangle \otimes |\varphi^-(\boldsymbol{k}_e)\rangle \otimes |\chi^-(\boldsymbol{k}_{se})\rangle \qquad (\boldsymbol{k}_{se} = \tfrac{1}{2}(\boldsymbol{k}_s - \boldsymbol{k}_e)), \tag{27}$$

where $|\varphi^-(\boldsymbol{k}_s)\rangle$ and $|\varphi^-(\boldsymbol{k}_e)\rangle$ are the Coulomb waves describing outgoing electrons moving in the field of the proton. The electron-electron correlation factor $|\chi^-(\boldsymbol{k}_{se})\rangle$ is determined through

$$|\boldsymbol{k}_s\rangle \otimes |\boldsymbol{k}_e\rangle \otimes |\chi^-(\boldsymbol{k}_{se})\rangle = |\psi^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle,$$

where $|\psi^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle$ is the exact scattering state in the absence of the electron-proton interactions. The wave function (27) has the correct asymptotic behavior and gives

correct results in the limiting situations, where (i) the charge of one of the final-state particles is switched off and (ii) the electron-electron interaction is absent. Note that the BBK model yields the regularization function (B.7) as

$$R_{\mathrm{BBK}} = \exp(-\tfrac{1}{2}\pi\eta)\Gamma(1 - \mathrm{i}\eta_s)\Gamma(1 - \mathrm{i}\eta_e)\Gamma(1 - \mathrm{i}\eta_{se}). \tag{28}$$

The corresponding Gamow factor is then given by

$$\mathcal{G}_{\mathrm{BBK}} = \mathcal{G}(\eta_s)\mathcal{G}(\eta_e)\mathcal{G}(\eta_{se}) = \frac{2\pi\eta_s}{\mathrm{e}^{2\pi\eta_s} - 1}\frac{2\pi\eta_e}{\mathrm{e}^{2\pi\eta_e} - 1}\frac{2\pi\eta_{se}}{\mathrm{e}^{2\pi\eta_{se}} - 1}. \tag{29}$$

Like (24), this Gamow factor also treats the final-state particle pairs on equal footing.

The numerical calculations using the traditional PWBA and PWIA models have been performed in accordance with equations (26) and (20), respectively. As remarked in subsection 4.3, in the case of symmetric kinematics the RPWBA (25) and RPWIA (23) models are equivalent and therefore below the corresponding numerical results referred to as RPWBA/RPWIA. For a hydrogen target, the structure factor entering equations (20), (23), (25), and (26) is

$$\sum^{(\mathrm{av})} |F_{if}(\boldsymbol{q})|^2 = |\varphi_{1s}(q)|^2, \tag{30}$$

where $\varphi_{1s}(q)$ is the $1s$ state momentum-space wave function.

5.1. Numerical results and discussion

Figure 1 shows the numerical results for the symmetric noncoplanar kinematics utilized in the recent (e,2e) measurements on helium [3]. It can be seen that the RPWBA/RPWIA results are substantially larger in magnitude than the PWIA ones, which are the smallest in magnitude. This feature indicates an appreciable role of the choice of the Gamow factor in the kinematics under consideration. Interestingly, the PWBA and BBK results are close to each other both in magnitude and in shape. Though the BBK model is not exact, it takes into account those higher-order effects that are entirely neglected by the PWBA treatment. One might thus conclude that the higher-order contributions to the TDCS are subsidiary in the present case. However, this conclusion needs experimental verification, since marked discrepancies between the PWBA and PWB2 results are observed in figure 1. It should be remarked that the developed renormalized first-order theories give an opportunity to fit the exact TDCS by the proper choice of the Gamow factor. For example, setting (cf equation (24))

$$G(\eta) = 1$$

in equations (23) and (25), one obtains the traditional PWBA result and thus, as can be seen in figure 1, rather well reproduces the BBK results for the present kinematics. And the PWB2 results are satisfactorily reproduced in magnitude using the modified Gamow factor (24).

In figure 2 the traditional PWBA and PWIA and the RPWBA/RPWIA values are presented on a logarithmic scale. It can be seen that all three models exhibit
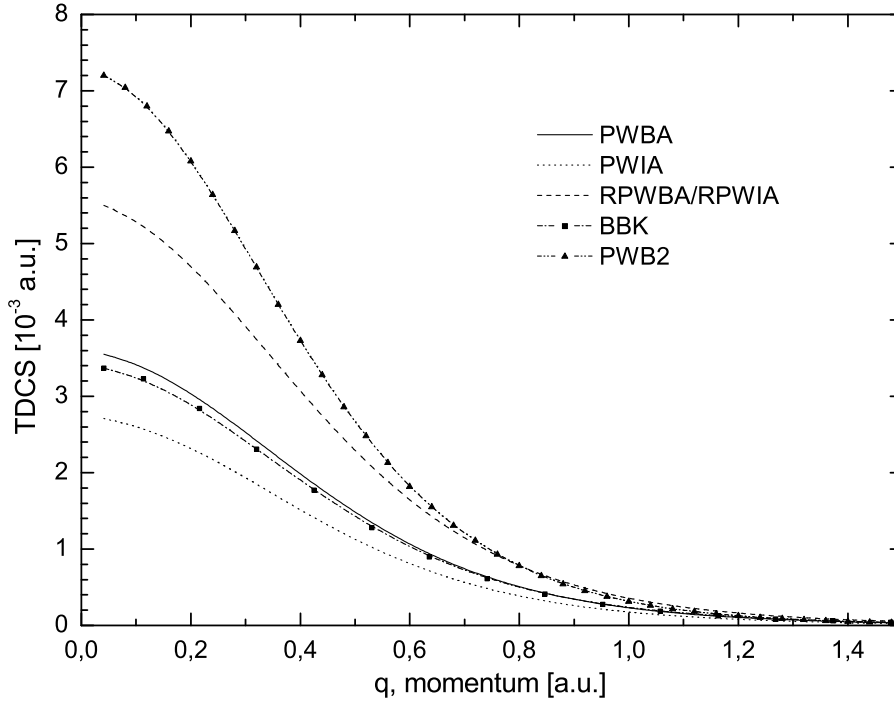
Figure 1. TDCS as a function of the absolute value of the recoil ion momentum in the symmetric noncoplanar kinematics ($E_s = E_e = 1000$ eV, $\theta_s = \theta_e = 45°$) of the recent (e,2e) experiments [3].

practically identical shapes for the TDCS. This feature is due to the almost constancy of the Sommerfeld parameters η_{se} and η, and hence of the Gamow factors (21) and (24), in the involved kinematical region. It should be noted that the value of the Gamow factor (29) is nearly the same as that of (24). This observation can be explained by the feature that the first-order expansions of (24) and (29) with respect to η_s, η_e, and η_{se} are identical. Another important observation is that, in contrast to the traditional Gamow factor (21), the modified Gamow factor (24) enhances the magnitude of the TDCS with respect to that in the conventional PWBA case. At the same time, all three first-order models are practically equivalent for description of the corresponding symmetric noncoplanar measurements provided that the latter are performed on a relative scale (see, for instance, [18]). This conclusion follows from the fact that in the case of the inspected first-order models the shape of the TDCS (the so-called momentum profile [1, 3, 4]) is almost fully determined by the structure factor (30).

The effect of the Gamow factor on the magnitude of TDCS in the considered geometry is shown in figure 3. As can be deduced from the figure, the RPWBA/RPWIA and the traditional PWIA values for the TDCS rather slowly converge to each other and ultimately to the traditional PWBA value upon the increase of the incident electron energy E_0. For $E_0 \sim 10$ keV, the RPWBA/RPWIA results are larger in magnitude than the traditional PWIA ones by a factor of ~ 1.5, and even in the region $E_0 \sim 100$ keV,
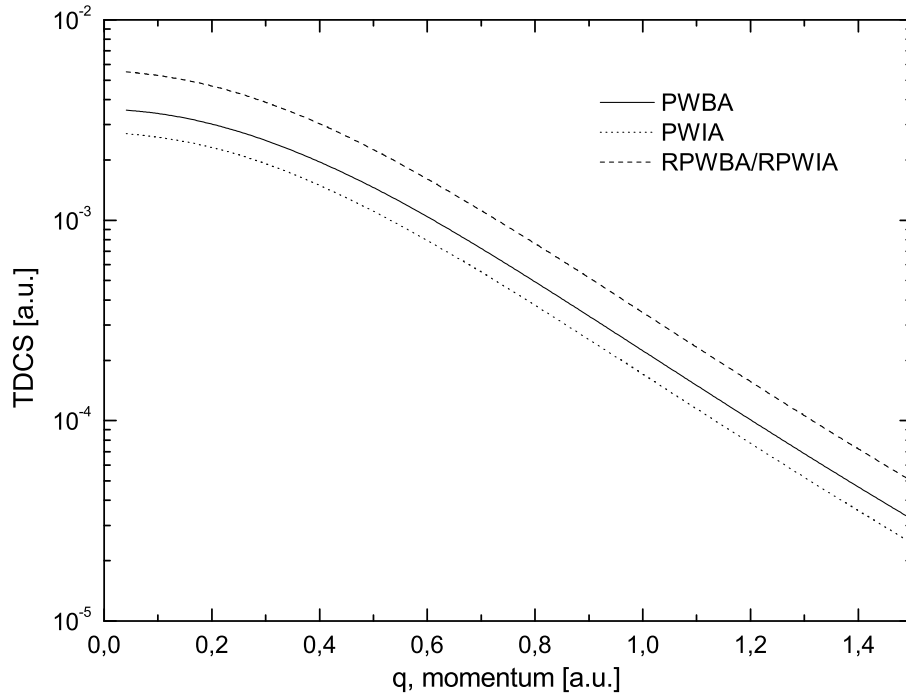
Figure 2. The first-order results for the TDCS. The kinematics is the same as in figure 1.

where one might expect relativistic effects to come on the scene, the relative difference between the results in magnitude is about 10%. These findings are in discord with an intuitive physical picture which assumes practical equivalence of the first-order models in the kinematics that approaches the classical ridge of a billiard-ball collision [2]. The discrepancy can be explained by the following factors: (i) the long-range Coulomb forces between the colliding electrons, as opposed to the contact-like forces between classical billiard balls, and (ii) the presence of the Coulomb field of the ion (this factor is relevant only to the RPWBA/RPWIA model).

6. Summary and conclusions

In summary, we have considered the electron-atom ionization process at large energy-momentum transfer and near the Bethe ridge. Proceeding from the plane wave Lippmann-Schwinger amplitude, which diverges on the energy shell, we have regularized the corresponding Born series. On this basis we have developed the correct, physical Born treatment whose lowest-order term amounts to the conventional PWBA. The RPWBA model has been formulated, which depends on the employed regularization procedure. We have shown that the PWIA can not be uniquely determined and therefore we have introduced the RPWIA model, in which the Gamow factor is determined by the choice of a regularization procedure. The numerical results for the symmetric
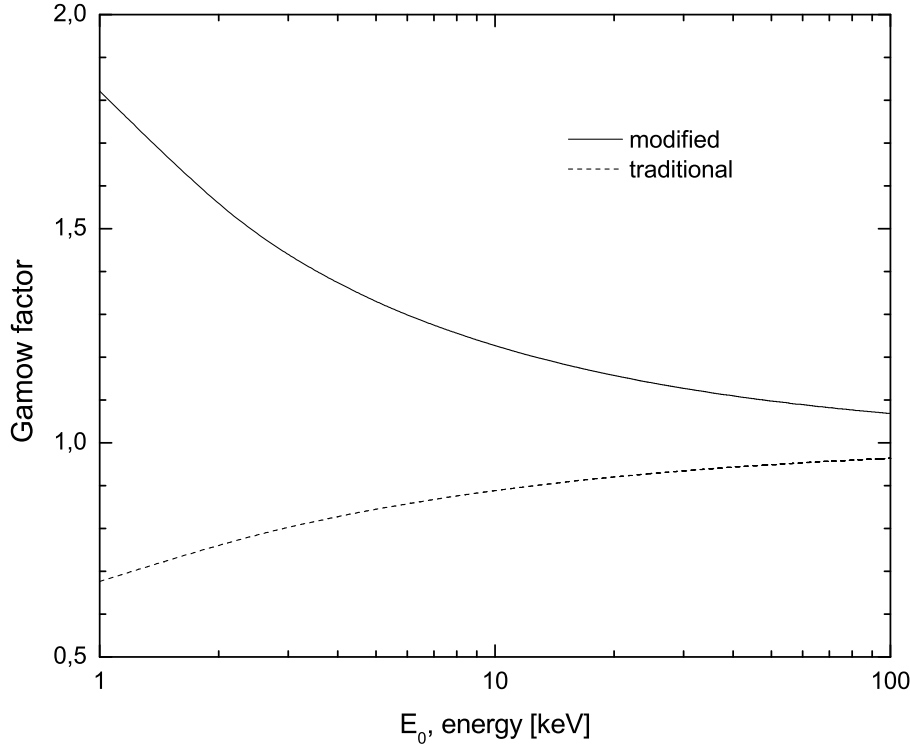
Figure 3. The traditional (21) and modified (24) Gamow factors as functions of the incident energy E_0 in the symmetric coplanar case ($E_s = E_e$, $\theta_s = \theta_e = 45°$, and $|\Delta\phi_{se}| = \pi$).

noncoplanar kinematics have been presented. It has been demonstrated that even at high electron energies (~ 10 keV) the magnitude of the TDCS is very sensitive to the choice of the Gamow factor.

We might expect the results of this work to be primarily important for theoretical treatments of absolute (e,2e) measurements in the nearly Bethe-ridge kinematics at large energy-momentum transfer and for further development of the EMS method [1]. The present theoretical consideration can be generalized to the case of ionization of an atom by a charged-particle impact, for example, to the cases of positron- and proton-atom ionization. Using the formulated RPWBA and RPWIA models with a properly modified Gamow factor, one can efficiently take into account the higher-order effects ignored by the traditional PWBA and PWIA models. In this connection, it should be noted that a consistent, rigorous treatment of the higher-order contributions to the ionization amplitude is realized by means of the developed plane wave Born series (12), which has an apparent advantageous feature: the value of any of its terms is, by definition, irrespective of the choice of a regularization procedure.

Acknowledgments

Appendix A. Divergencies of the Born series

To elucidate the origin of divergencies, let us examine the electron-electron part of the $n = 1$ term in (6)

$$\tilde{T}_{se}^{(1)} = \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \frac{\langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \boldsymbol{p}_s \boldsymbol{p}_e \Phi_f^{Z-1} \rangle}{E - p_s^2/2 - p_e^2/2 - \varepsilon_f - \mathrm{i}0} \langle \boldsymbol{p}_s \boldsymbol{p}_e | V_{se} | \boldsymbol{k}_s \boldsymbol{k}_e \rangle$$

$$= \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \frac{\langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \boldsymbol{k}_s - \boldsymbol{p}, \boldsymbol{k}_e + \boldsymbol{p}, \Phi_f^{Z-1} \rangle}{(\boldsymbol{k}_s - \boldsymbol{k}_e) \cdot \boldsymbol{p} - p^2 - \mathrm{i}0} \frac{4\pi}{p^2}. \tag{A.1}$$

It can be seen that the integrand has a pronounced singularity at the point $\boldsymbol{p} = 0$ which physically corresponds to elastic rescattering in the forward direction. This feature makes the integral (A.1) divergent. The same argument applies to the electron-ion parts of the $n = 1$ term, since for the static matrix elements of V_s and V_e we have:

$$\langle \boldsymbol{k}_s \pm \boldsymbol{p}, \Phi_f^{Z-1} | V_s | \boldsymbol{k}_s \Phi_f^{Z-1} \rangle = \langle \boldsymbol{k}_e \pm \boldsymbol{p}, \Phi_f^{Z-1} | V_e | \boldsymbol{k}_e \Phi_f^{Z-1} \rangle \simeq -\frac{4\pi}{p^2} \qquad (p \to 0).$$

Clearly, in the case $n \geq 2$ we encounter even stronger divergencies because the corresponding Born terms contain multiple elastic rescattering in the forward direction.

In the case of (8), the electron-electron part of the $n = 1$ term takes the form (cf (A.1))

$$\tilde{T}_{se}^{(1)}(\Delta) = \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \frac{\langle \boldsymbol{k}_0 \Phi_i^Z | V_i | \boldsymbol{k}_s - \boldsymbol{p}, \boldsymbol{k}_e + \boldsymbol{p}, \Phi_f^{Z-1} \rangle}{\Delta + (\boldsymbol{k}_s - \boldsymbol{k}_e) \cdot \boldsymbol{p} - p^2 - \mathrm{i}0} \frac{4\pi}{p^2}, \tag{A.2}$$

where the singularity in the integrand at the point $\boldsymbol{p} = 0$ is removed (note that $\mathrm{d}\boldsymbol{p} = p^2 \mathrm{d}p \, \mathrm{d}\Omega_p$) and thereby the integral does not diverge. Specifically, in the case $\Delta \to 0$ we have [5]

$$\tilde{T}_{se}^{(1)}(\Delta) \sim -\mathrm{i}\eta_{se} T^{\mathrm{PWBA}} \ln \Delta.$$

Appendix B. Regularization procedure

Below we describe a possible recipe for factoring out $\Delta^{-\mathrm{i}\eta}$ in equation (8) and then taking the on-shell limit in equation (9). It consists in presenting the Green's operator (4) in the form

$$G_0^-(E) = \sum_{f'} \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \frac{|\boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1}\rangle \langle \boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1}|}{E - p_s^2/2 - p_e^2/2 - \varepsilon_{f'} - \mathrm{i}0} = \mathcal{G}_0^-(E) + \mathcal{F}_0^-(E), \tag{B.1}$$

where $\mathcal{G}_0^-(E)$ is the regularized Green's operator and

$$\mathcal{F}_0^-(E) = \sum_{f'} \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \frac{|\boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1}\rangle \langle \boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1}|}{E - p_s^2/2 - p_e^2/2 - \varepsilon_{f'} - \mathrm{i}0} \tag{B.2}$$

is the Green's operator component which is responsible for divergencies. Using (B.1) and (B.2), we obtain the off-shell Born series (8) in the factorized form

$$\tilde{T}(\Delta) = P_R(\Delta)\tilde{T}_R(\Delta), \tag{B.3}$$

where

$$\tilde{T}_R(\Delta) = \sum_{n=0}^{\infty} \tilde{T}_R^{(n)}(\Delta) \equiv T^{\mathrm{PWBA}} + \sum_{n=1}^{\infty} \tilde{T}_R^{(n)}(\Delta),$$

$$P_R(\Delta) = \sum_{n=0}^{\infty} P_R^{(n)}(\Delta) \equiv 1 + \sum_{n=1}^{\infty} P_R^{(n)}(\Delta),$$

with

$$\tilde{T}_R^{(n)}(\Delta) = \langle \boldsymbol{k}_0 \Phi_i^Z | V_i [\mathcal{G}_0^-(E)V]^n | \boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1} \rangle,$$

$$P_R^{(n)}(\Delta) = \sum_{f'} \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \langle \boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1} | [G_0^-(E)V]^n | \boldsymbol{k}_s \boldsymbol{k}_e \Phi_f^{Z-1} \rangle.$$

Taking into account that

$$1 + \sum_{n=1}^{\infty} [G_0^-(E)V]^n = 1 + G^-(E)V$$

and using (5), we get

$$\lim_{\Delta \to 0} P_R(\Delta) = \sum_{f'} \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \langle \boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1} | \tilde{\Psi}_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e) \rangle. \tag{B.4}$$

The on-shell limit (B.4) does not exist, since the Lippmann-Schwinger total scattering state $|\tilde{\Psi}_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e)\rangle$ is not physical. Using the results of Shablov *et al* [7, 8], we deduce that

$$P_R(\Delta \to 0) = \Delta^{-\mathrm{i}\eta} \exp(\tfrac{1}{2}\pi\eta + \mathrm{i}A)\Gamma(1 + \mathrm{i}\eta)$$

$$\times \sum_{f'} \int \frac{\mathrm{d}\boldsymbol{p}_s}{(2\pi)^3} \frac{\mathrm{d}\boldsymbol{p}_e}{(2\pi)^3} \langle \boldsymbol{p}_s \boldsymbol{p}_e \Phi_{f'}^{Z-1} | \Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e) \rangle. \tag{B.5}$$

Inserting (B.3) into (9) and using (B.5), we obtain the physical amplitude as

$$T = R\tilde{T}_R, \qquad \text{where } \tilde{T}_R = \sum_{n=0}^{\infty} \tilde{T}_R^{(n)} \equiv T^{\mathrm{PWBA}} + \sum_{n=1}^{\infty} \tilde{T}_R^{(n)}. \tag{B.6}$$

Here $\tilde{T}_R^{(n)} = \lim_{\Delta \to 0} \tilde{T}_R^{(n)}(\Delta)$ is the regularized on-shell Born term. The regularization function R is given by

$$R = \sum_{f'} \langle \delta(\boldsymbol{r}_s)\delta(\boldsymbol{r}_e)\Phi_{f'}^{Z-1} | \Psi_f^-(\boldsymbol{k}_s, \boldsymbol{k}_e) \rangle, \tag{B.7}$$

where $\delta(\boldsymbol{r})$ designates Dirac's delta function. The function (B.7) has the following obvious property: $R = 1$ if $\tilde{\boldsymbol{\eta}} = 0$, where $\tilde{\boldsymbol{\eta}} = (\eta_s, \eta_e, \eta_{se})$.

Note that the above recipe for regularization is only one among an infinite number of possible regularization procedures and, in general, one obtains different regularization

functions for different regularization procedures. It means that while the product $R\tilde{T}_R = T$ (B.6) is an algoristic quantity, the factors R and $\tilde{T}_R$ are not, i.e. $R\tilde{T}_R = \mathcal{R}\tilde{T}_\mathcal{R}$, where $\mathcal{R}$ ($\mathcal{R} = 1$ if $\tilde{\boldsymbol{\eta}} = 0$) and $\tilde{T}_\mathcal{R}$ corresponds to an alternative regularization procedure. For example, there is such regularization procedure that yields $\mathcal{R} = 1$ for any value of $\tilde{\boldsymbol{\eta}}$. To illustrate this statement, we expand R in the Taylor series with respect to the components of $\tilde{\boldsymbol{\eta}}$ and notice that $\tilde{T}_R^{(n)} \propto \tilde{\eta}^n$. We have

$$R\tilde{T}_R = \sum_{n=0}^{\infty} \frac{(\tilde{\boldsymbol{\eta}} \cdot \boldsymbol{\nabla}_{\tilde{\eta}=0})^n R}{n!} \sum_{m=0}^{\infty} \tilde{T}_R^{(m)} = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{(\tilde{\boldsymbol{\eta}} \cdot \boldsymbol{\nabla}_{\tilde{\eta}=0})^{n-m} R}{(n-m)!} \tilde{T}_R^{(m)}$$

$$= \sum_{n=0}^{\infty} \tilde{T}_{\mathcal{R}=1}^{(n)} = \tilde{T}_{\mathcal{R}=1}, \tag{B.8}$$

where it is supposed that the operator

$$\tilde{\boldsymbol{\eta}} \cdot \boldsymbol{\nabla}_{\tilde{\eta}=0} = \eta_s \left(\frac{\partial}{\partial \eta_s} \right)_{\tilde{\eta}=0} + \eta_e \left(\frac{\partial}{\partial \eta_e} \right)_{\tilde{\eta}=0} + \eta_{se} \left(\frac{\partial}{\partial \eta_{se}} \right)_{\tilde{\eta}=0}$$

acts only on the regularization function R, and $(\tilde{\boldsymbol{\eta}} \cdot \boldsymbol{\nabla}_{\tilde{\eta}=0})^0 R = R|_{\tilde{\eta}=0} = 1$. As can be deduced, $\tilde{T}_{\mathcal{R}=1}^{(n)} \propto \tilde{\eta}^n$ and $\tilde{T}_{\mathcal{R}=1}^{(0)} = \tilde{T}_R^{(0)} \equiv T^{\text{PWBA}}$.

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